Triisopropanolamine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.89e-01

Global applicability domain: Inside

Local applicability domain index: 4.53e-01

Confidence level: 7.30e-01

Nearest Neighbors from the Training Set

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Diisopropanolamine	Methyl N-acetyl-L-leucinate	2-(tert-Butylamino)ethanol
Measured: -0.820	**Measured:** 0.84	**Measured:** 0.41
Predicted: -0.672	**Predicted:** 6.15e-01	**Predicted:** 6.72e-01